10526940elected

Search elected species and claim 1

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:02:23 ON 07 MAR 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 09:02:32 ON 07 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 MAR 2007 HIGHEST RN 924962-30-1
DICTIONARY FILE UPDATES: 5 MAR 2007 HIGHEST RN 924962-30-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

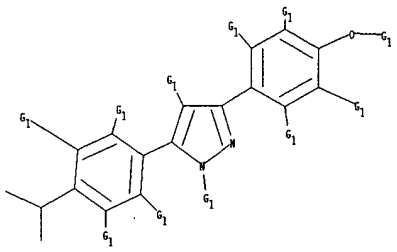
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

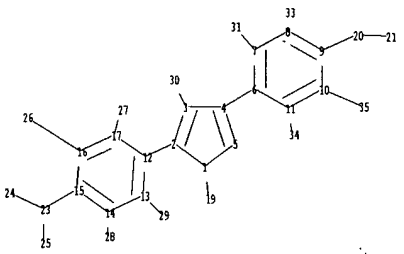
http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526940elected.str

Karen Cheng

10526940elected





chain nodes :
19 20 21 23 24 25 26 27 28 29 30 31 33 34 35
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
1-19 2-12 3-30 4-6 7-31 8-33 9-20 10-35 11-34 13-29 14-28 15-23 16-26
17-27 20-21 23-24 23-25
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14
14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 1-19 3-30 4-5 7-31 8-33 9-20 10-35 11-34 13-29 14-28 16-26
17-27 20-21
exact bonds :
2-3 2-12 3-4 4-6 15-23 23-24 23-25
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 12 :

G1:H,CH3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS
21:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 31:CLASS 33:CLASS 34:CLASS 35:CLASS

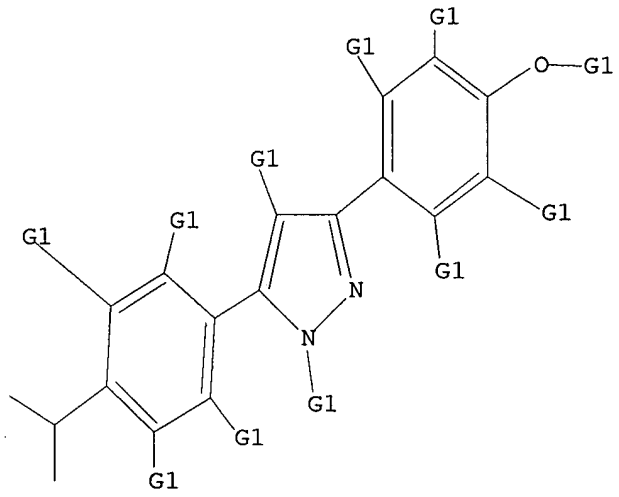
L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS

Karen Cheng

10526940elected

L1 STR



G1 H,Me

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 09:02:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 22607 TO ITERATE

100.0% PROCESSED 22607 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L2 0 SEA SSS FUL L1

=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'STNGUIDE' ENTERED AT 09:03:03 ON 07 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 2, 2007 (20070302/UP).

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.12	172.43

FILE 'REGISTRY' ENTERED AT 09:04:04 ON 07 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Karen Cheng

10526940elected

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 MAR 2007 HIGHEST RN 924962-30-1
DICTIONARY FILE UPDATES: 5 MAR 2007 HIGHEST RN 924962-30-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

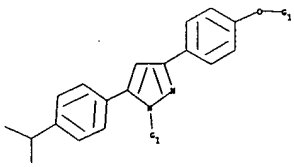
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

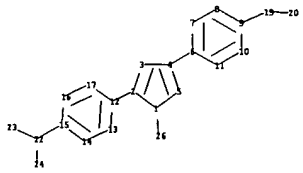
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526940electeda.str





chain nodes :
19 20 22 23 24 26
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
1-26 2-12 4-6 9-19 15-22 19-20 22-23 22-24
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 1-26 4-5 9-19 19-20
exact bonds :
2-3 2-12 3-4 4-6 15-22 22-23 22-24
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17

Karen Cheng

10526940elected

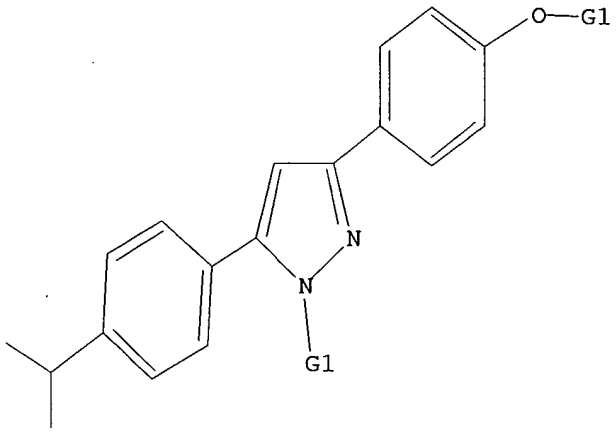
isolated ring systems :
containing 1 : 6 : 12 :

G1:H,CH3

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS
22:CLASS 23:CLASS 24:CLASS 26:CLASS

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR



G1 H,Me

Structure attributes must be viewed using STN Express query preparation.

=> s l3 full
FULL SEARCH INITIATED 09:04:19 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 22607 TO ITERATE

100.0% PROCESSED 22607 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L4 0 SEA SSS FUL L3

=> fil stng
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 344.53

FILE 'STNGUIDE' ENTERED AT 09:04:23 ON 07 MAR 2007

Karen Cheng

10526940elected

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 2, 2007 (20070302/UP).

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.06	344.59

FILE 'REGISTRY' ENTERED AT 09:05:09 ON 07 MAR 2007

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 MAR 2007 HIGHEST RN 924962-30-1
DICTIONARY FILE UPDATES: 5 MAR 2007 HIGHEST RN 924962-30-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

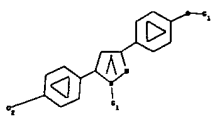
TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

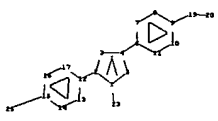
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526940electedb.str





Karen Cheng

10526940elected

chain nodes :
19 20 23 25
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
1-23 2-12 4-6 9-19 15-25 19-20
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14
14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 1-23 4-5 9-19 15-25 19-20
exact bonds :
2-3 2-12 3-4 4-6
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 12 :

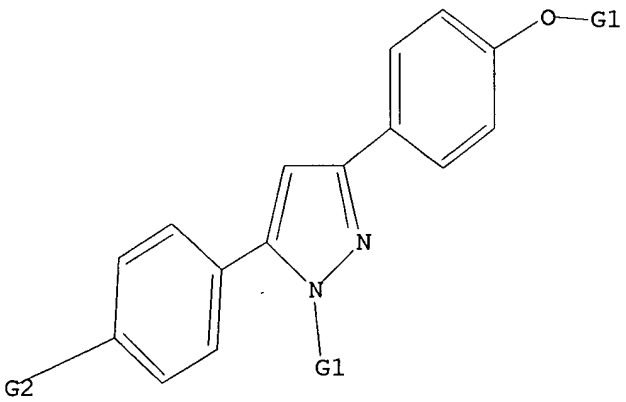
G1:H,CH3

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS
23:CLASS 25:CLASS

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR



G1 H,Me

G2 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Karen Cheng

10526940elected

Structure attributes must be viewed using STN Express query preparation.

=> s l5 full
FULL SEARCH INITIATED 09:05:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 36786 TO ITERATE

100.0% PROCESSED 36786 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.01

L6 14 SEA SSS FUL L5

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.10 516.69

FILE 'CAPLUS' ENTERED AT 09:05:35 ON 07 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 7 Mar 2007 VOL 146 ISS 11
FILE LAST UPDATED: 6 Mar 2007 (20070306/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

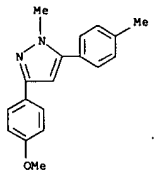
http://www.cas.org/infopolicy.html

=> s l6
L7 3 L6

=> d ibib abs hitstr tot

Karen Cheng

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:660707 CAPLUS
DOCUMENT NUMBER: 145:292939
TITLE: Reaction of N-Monosubstituted Hydrazones with Nitroolefins: A Novel Regioselective Pyrazole Synthesis
AUTHOR(S): Deng, Xiaohu; Mani, Neelakandha S.
CORPORATE SOURCE: Department of Drug Discovery, Johnson & Johnson Pharmaceutical R & D LLC, San Diego, CA, 92121, USA
SOURCE: Organic Letters (2006), 8(16), 3505-3508
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A novel regioselective synthesis of substituted pyrazoles from N-monosubstituted hydrazones and nitroolefins is described. The reaction is performed in a one-pot manner and the yields range from moderate to excellent. A key nitropyrazolidine intermediate is characterized and a plausible mechanism is proposed.
IT 908329-93-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(one-pot regioselective synthesis of substituted pyrazoles from N-monosubstituted hydrazones and nitroolefins)
RN 908329-93-1 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-1-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

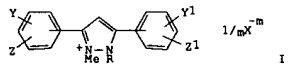
L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:116915 CAPLUS
DOCUMENT NUMBER: 84:116915
TITLE: Pyrazolium fungicides
INVENTOR(S): Walworth, Bryant L.
PATENT ASSIGNEE(S): American Cyanamid Co., USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3930011	A	19751230	US 1975-546654	19750203
ZA 7507951	A	19761229	ZA 1975-7951	19751222
IL 48708	A	19780731	IL 1975-48708	19751223
AU 7587903	A	19770630	AU 1975-87903	19751224
AU 500653	B2	19790531		
GB 1534866	A	19781206	GB 1975-53214	19751230
CA 1058517	A1	19790717	CA 1976-243287	19760109
NL 7600700	A	19760805	NL 1976-700	19760123
DK 7600296	A	19760804	DK 1976-296	19760126
DK 139833	C	19791001		
DK 139833	B	19790430		
FI 7600174	A	19760804	FI 1976-174	19760126
FI 59194	B	19810331		
FI 59194	C	19810710		
DE 2602964	A1	19760805	DE 1976-2602964	19760127
CS 199651	B2	19800731	CS 1976-580	19760129
BE 838171	A4	19760802	BE 1976-164007	19760202
SE 7601095	A	19760803	SE 1976-1095	19760202
SE 420888	B	19811109		
SE 420888	C	19820218		
NO 7600343	A	19760804	NO 1976-343	19760202
NO 145039	B	19810921		
NO 145039	C	19820104		
BR 7600646	A	19760831	BR 1976-646	19760202
CH 594354	A5	19780113	CH 1976-1243	19760202
AT 347178	B	19781211	AT 1976-697	19760202
SU 644359	A3	19790125	SU 1976-2319208	19760202
FR 2298949	A2	19760827	FR 1976-2975	19760203
FR 2298949	B2	19790330		
JP 51104031	A	19760914	JP 1976-10777	19760203
DD 124703	A6	19770309	DD 1976-191070	19760203

PRIORITY APPLN. INFO.: US 1971-209448 A 19711217
US 1972-271424 A 19720713
GB 1972-55680 A 19721201
US 1975-546654 A 19750203

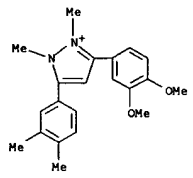
GI

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



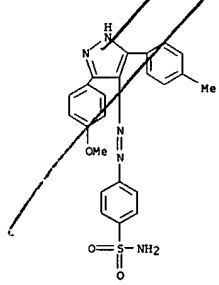
I

AB Dialkyldiphenylpyrazolium salts I (R=alkyl, allyl, propynyl, ethylcarboxymethyl, Ph, or PhCH2; Y,Y',Z, and Z'=H, halogen, C1-4 alkyl or alkoxy; X=mono- or divalent anion; m = 1 or 2) were effective as fungicides. For example, 1,2-dimethyl-3,5-diphenylpyrazolium methyl sulfate [43222-48-6] was effective for control of Phytophthora infestans on tomato, Piricularia oryzae on rice, and Venturia inaequalis on apple. The synthesis of I is described.
IT 58538-38-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and fungicidal activity of)
RN 58538-38-8 CAPLUS
CN 1H-Pyrazolium, 3-(3,4-dimethoxyphenyl)-5-(3,4-dimethylphenyl)-1,2-dimethyl-, iodide (9CI) (CA INDEX NAME)



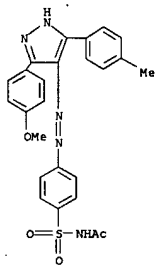
● I⁻

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1976:105469 CAPLUS
DOCUMENT NUMBER: 84:105469
TITLE: Studies in heterocyclic compounds. Part VI. Synthesis and antibacterial activity of some 3,5-diaryl-4-(N-substituted p-sulfamoylphenylazo)pyrazoles
AUTHOR(S): Saharia, G. S.; Sharma, H. R.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, India
SOURCE: Indian Journal of Pharmacy (1975), 37(6), 147-50
CODEN: IJPAAO; ISSN: 0019-5472
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Sixty-two pyrazoles I (R = H, Ac, Ph, substituted phenyl, pyrimidyl, etc.; R1 = H, OMe; R2 = H, Ph, p-MeC6H4, p-O2NC6H4), nearly all of which showed antibacterial activity against Escherichia coli and none of them against Staphylococcus aureus were prepared by reaction of p-MeC6H4COCH(N:NC6H4SO2NHR-p)COC6H4R1-p with R2NHNH2 in AcOH or AcOH-EtOH at reflux. I (R1 = OMe) were more active than I (R1 = H).
IT 58524-22-4P 58524-23-5P 58524-24-6P
58524-25-7P 58524-26-8P 58524-27-9P
58524-28-0P 58524-29-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antibacterial activity of)
RN 58524-22-4 CAPLUS
CN Benzenesulfonamide, 4-[[3-(4-methoxyphenyl)-5-(4-methylphenyl)-1H-pyrazol-4-yl]azo]- (9CI) (CA INDEX NAME)

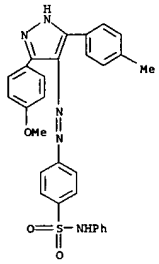


RN 58524-23-5 CAPLUS
CN Acetamide, N-[[4-[[3-(4-methoxyphenyl)-5-(4-methylphenyl)-1H-pyrazol-4-yl]azo]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



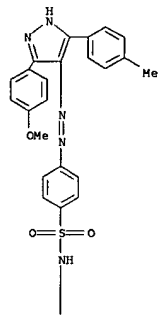
RN 58524-24-6 CAPLUS
CN Benzenesulfonamide, 4-[[3-(4-methoxyphenyl)-5-(4-methylphenyl)-1H-pyrazol-4-yl]azo]-N-phenyl- (9CI) (CA INDEX NAME)



RN 58524-25-7 CAPLUS
CN Benzenesulfonamide, N-(4-chlorophenyl)-4-[[3-(4-methoxyphenyl)-5-(4-methylphenyl)-1H-pyrazol-4-yl]azo]- (9CI) (CA INDEX NAME)

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A

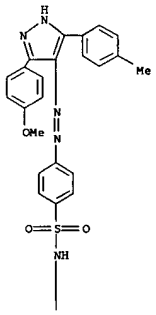


PAGE 2-A

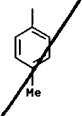
RN 58524-26-8 CAPLUS
CN Benzenesulfonamide, 4-[[3-(4-methoxyphenyl)-5-(4-methylphenyl)-1H-pyrazol-4-yl]azo]-N-(4-methylphenyl)- (9CI) (CA INDEX NAME)

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



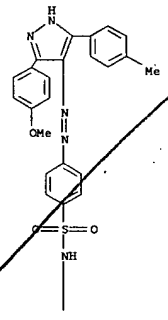
PAGE 2-A



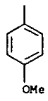
RN 58524-27-9 CAPLUS
CN Benzenesulfonamide, N-(4-methoxyphenyl)-4-[[3-(4-methoxyphenyl)-5-(4-methylphenyl)-1H-pyrazol-4-yl]azo]- (9CI) (CA INDEX NAME)

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



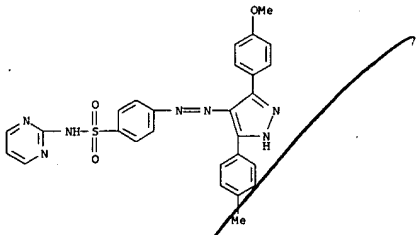
PAGE 2-A



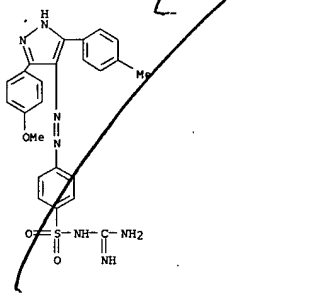
RN 58524-28-0 CAPLUS
CN Benzenesulfonamide, 4-[[3-(4-methoxyphenyl)-5-(4-methylphenyl)-1H-pyrazol-4-yl]azo]-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

10526940elected

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 58524-29-1 CAPLUS
CN Benzenesulfonamide, N-(aminoiminomethyl)-4-[[3-(4-methoxyphenyl)-5-(4-methylphenyl)-1H-pyrazol-4-yl]azo]- (9CI) (CA INDEX NAME)



Karen Cheng

10526940elected

=> fil stng
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.40	576.04

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

FILE 'STNGUIDE' ENTERED AT 09:11:55 ON 07 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY, JAPAN SCIENCE
AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Mar 2, 2007 (20070302/UP).

=> fil reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.54	576.58

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

FILE 'REGISTRY' ENTERED AT 09:17:36 ON 07 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 5 MAR 2007 HIGHEST RN 924962-30-1
DICTIONARY FILE UPDATES: 5 MAR 2007 HIGHEST RN 924962-30-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

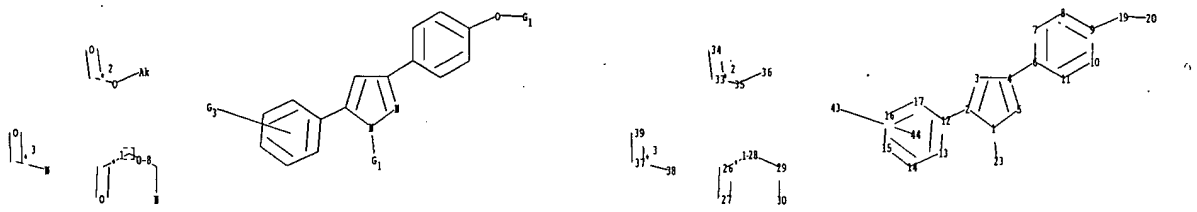
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10526940electedc.str

Karen Cheng

10526940elected



chain nodes :
19 20 23 26 27 28 29 30 33 34 35 36 37 38 39 43
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
1-23 2-12 4-6 9-19 19-20 26-28 26-27 28-29 29-30 33-35 33-34 35-36
37-38 37-39
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14
14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 1-23 4-5 9-19 19-20 26-27 29-30 33-35 33-34 35-36 37-38 37-39
exact bonds :
2-3 2-12 3-4 4-6 26-28 28-29
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 12 :

G1:H,CH3

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3:H,Ak,X,[*1],[*2],[*3]

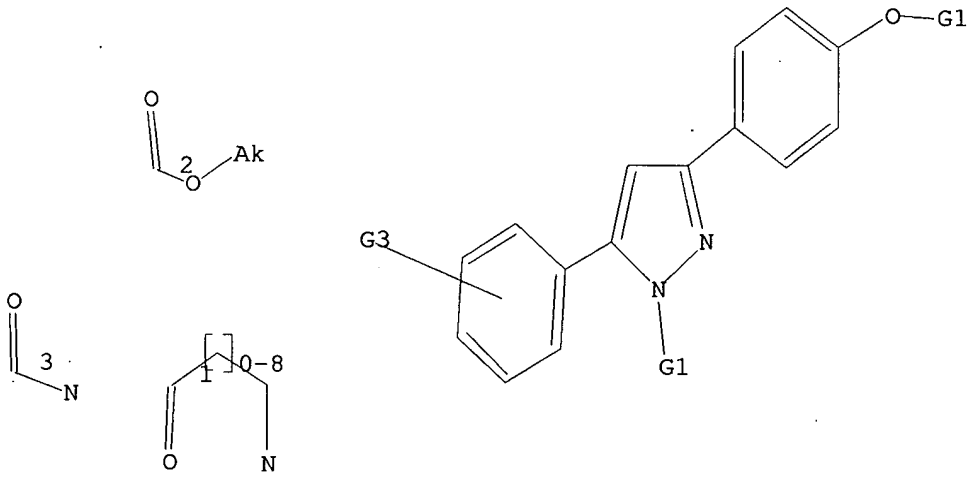
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS
23:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 33:CLASS 34:CLASS
35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 43:CLASS 44:Atom

L11 STRUCTURE UPLOADED

Karen Cheng

10526940elected

=> d
L11 HAS NO ANSWERS
L11 STR



G1 H,Me

G2 Me,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G3 H,Ak,X,[@1],[@2],[@3]

Structure attributes must be viewed using STN Express query preparation.

=> s l11 full
FULL SEARCH INITIATED 09:17:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 106460 TO ITERATE

100.0% PROCESSED 106460 ITERATIONS 225 ANSWERS
SEARCH TIME: 00.00.02

L12 225 SEA SSS FUL L11

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	748.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

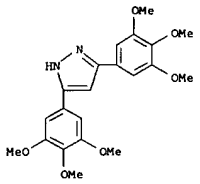
FILE 'CAPLUS' ENTERED AT 09:18:02 ON 07 MAR 2007

Karen Cheng

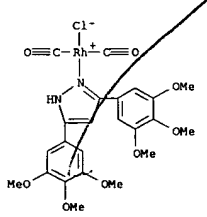
L13 ANSWER 1 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1194755 CAPLUS
DOCUMENT NUMBER: 146:154646
TITLE: Supramolecular Structures and Columnar Mesophase Induction in Nondiscoid Pyrazoles by Complexation to Rhodium(I)
AUTHOR(S): Gimenez, Raquel; Elduque, Anabel; Lopez, Jose Antonio; Barbera, Joaquin; Cavero, Emma; Lantero, Ignacio; Oro, Luis A.; Serrano, Jose Luis
CORPORATE SOURCE: Departamento de Quimica Organica and Departamento de Quimica Inorganica, Facultad de Ciencias-Instituto de Ciencia de Materiales de Aragon, Universidad de Zaragoza-CSIC, Zaragoza, 50009, Spain
SOURCE: Inorganic Chemistry (2006), 45(25), 10363-10370
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several new cis-[RhCl(CO)2(Ln)] complexes were prepared using different polycatenar pyrazole ligands (Ln) to obtain columnar liquid crystalline arrangements. The topol. of the ligand plays an essential role, and a mesophase is induced at room temperature from a nonmesogenic pyrazole only when it is sym. substituted with six decyloxy chains. The single-crystal structure of a methoxy-substituted analog, 3,5-bis(3,4,5-trimethoxyphenyl)pyrazole, is formed by globular tetrameric structures held together by H-bonding. However, parallel dimers are present in the corresponding cis-chlorodicarbonylrhodium(I) complex, a situation that explains the induction of a columnar mesophase in the decyloxy-substituted complex. The XRD pattern of the mesophase is consistent with a hexagonal symmetry in which the columns are formed by mols. assembled in an antiparallel mode. The crystal-to-mesophase transition was also detected by spectroscopic techniques as a shift in the IR carbonyl stretching bands and the appearance of a charge-transfer band in the absorption spectrum with thermochromic behavior.

IT 851729-28-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of nondiscoid rhodium(I) pyrazole complexes)
RN 851729-28-7 CAPLUS
CN 1H-Pyrazole, 3,5-bis(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



L13 ANSWER 1 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



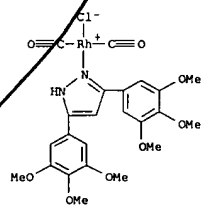
REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 1 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 918870-13-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure)
RN 918870-13-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 918870-10-7
CMF C23 H24 Cl N2 O8 Rh
CCI CCS



CM 2

CRN 75-09-2
CMF C H2 Cl2

IT 918870-10-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, melting enthalpy and columnar mesophase induction in nondiscoid rhodium(I) pyrazole complexes)
RN 918870-10-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

L13 ANSWER 2 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1167135 CAPLUS
DOCUMENT NUMBER: 146:81826
TITLE: Synthesis of some new pyrazoloquinazolinone and quinazolinone derivatives
AUTHOR(S): El-Khamry, A. A.; Shiba, S. A.; Shalaby, A. A.; Abd Alaha, A. A.
CORPORATE SOURCE: Chemistry Department, Faculty of Science, Ain Shams University, Cairo, Egypt
SOURCE: Journal of Heterocyclic Chemistry (2006), 43(5), 1189-1193
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

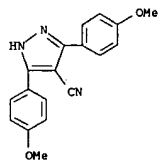
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The benzoxazinone derivative 2-(6,8-dibromo-4-oxo-4H-benzo[d]-1,3-oxazin-2-yl)-3-(4-methoxyphenyl)acrylonitrile was used as a starting material for preparation of the pyrazoloquinazolinone and quinazolinone derivs. Under different conditions the benzoxazinone I was reacted with hydrazine hydrate to provide the pyrazolocarbonitrile derivative and the azine derivative and/or the pyrazoloquinazoline derivative II. When the pyrazoloquinazoline derivative was conducted to react either with Et acetoacetate or Ac2O/AcOH mixture or phthalic anhydride/acetic acid mixture, the pyrazoloquinazoline carbonitrile, pyrazolo-quinazoline acetate or the pyrazoloquinazolinone derivative were formed resp. When the benzoxazinone was reacted with phenylhydrazine, a mixture of the quinazolinone derivative III and the hydrazone derivative were obtained. The benzoxazinone derivative was found also to react with benzylamine in ethanol or without solvent to give the quinazolinone derivative IV or the quinazolinedione resp. Fusion of the benzoxazinone with ammonium acetate yielded the quinazolinone, which was methylated to give the N-Me quinazolinone and sulfated to the thioxyquinazoline derivative In addition, the reaction of the benzoxazinone with formamide gave the N-formylquinazoline derivative

IT 917508-81-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of bis(methoxyphenyl)cyanopyrazole and bis(methoxybenzylidene)hydrazine via hydrazinolysis of [(dibromo)oxobenzoxazinyl](methoxyphenyl)acrylonitrile)
RN 917508-81-7 CAPLUS
CN 1H-Pyrazole-4-carbonitrile, 3,5-bis(4-methoxyphenyl)- (CA INDEX NAME)

Karen Cheng

L13 ANSWER 2 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

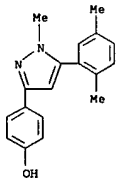
L13 ANSWER 3 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

(un)substituted aminocarbonyl, alkoxycarbonyl, etc., D and L, and Q and Y may link together to form a N/S-heterocyclyl ring, with limitations] and pharmaceutically acceptable salts thereof were prepd. as anticancer agents. For instance, treatment of 5'-chloro-2'-hydroxyacetophenone with 3-cyanobenzoyl chloride followed by cyclization with hydrazine hydrate gave diphenylpyrazole II. This product showed cell growth inhibition with IC50 of 0.23 μg/mL against MCF-7 cells and 0.066 μg/mL against MDA-MB-453 cells, resp. Therefore, the invented compds. and their pharmaceutical compns. are useful for the treatment of various cancer, such as breast cancer and lung cancer.

IT 362006-35-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(reference; preparation of diphenylpyrazoles as antitumor agents)

RN 362006-35-7 CAPLUS

CN Phenol, 4-[5-(2,5-dimethylphenyl)-1-methyl-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

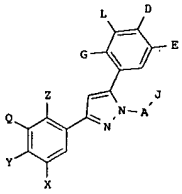
L13 ANSWER 3 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1095978 CAPLUS
DOCUMENT NUMBER: 145:438611
TITLE: Preparation of 3,5-diphenylpyrazoles as antitumor agents
INVENTOR(S): Kuroiwa, Shunsuke; Maruyama, Sakiko; Suzuki, Yoshikazu; Yamazaki, Hiroko
PATENT ASSIGNEE(S): Nippon Kayaku Kabushiki Kaisha, Japan
SOURCE: PCT Int. Appl., 45pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

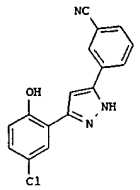
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006109680	A1	20061019	WO 2006-JP307346	20060406

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: JP 2005-110717 A 20050407
OTHER SOURCE(S): MARPAT 145:438611
GI



I



II

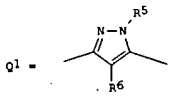
AB Title compds. I [wherein A = H, carbonyl or sulfonyl; J = (un)substituted alkyl or amino; G, Z = H, OH, alkoxy, etc.; D, E, L, Q, X, Y = H,

L13 ANSWER 4 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN

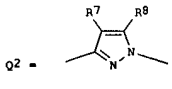
ACCESSION NUMBER: 2006:1089202 CAPLUS
DOCUMENT NUMBER: 145:439502
TITLE: Epoxy resin compositions, their epoxides having low melting point, and prepregs therewith
INVENTOR(S): Inoue, Kazuya; Hibino, Hiroaki
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 22pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006282531	A	20061019	JP 2005-101698	20050331

PRIORITY APPLN. INFO.: JP 2005-101698 20050331
GI



Q1 =



Q2 =

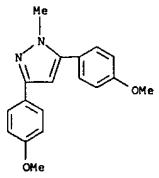
AB The epoxides are G2-p-C6H2R1R2Y-p-C6H2R3R4G [G = glycidyl; R1-R4 = H, halo, C1-8 alkyl(oxy), CN, NO2; Y = Q1, Q2 (R5 = H, C1-8 alkyl; R6-R8 = H, C1-8 alkyl, halo, CN, NO2; Z = single bond, O, C1-8 alkylene)]. Thus, 5 g 4-methoxyacetophenone was reacted with 5.5 g Me 4-methoxybenzoate to give 1,3-bis(4-methoxyphenyl)propane-1,3-dione in 83% yield, which was reacted with methylhydrazine, hydrolyzed, and reacted with epichlorohydrin in the presence of tetrabutylammonium bromide to give 3,5-bis[4-(oxiranylmethoxy)phenyl]-1-methylpyrazole (I; m.p. 127°) in 91% yield. Then, I was reacted with diaminodiphenylmethane, poured in a mold, and kept at 145-155° and then at 180° to give a cured resin.

IT 43222-90-8P 912804-13-8P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(pyrazolyl group-containing epoxy compds. and their compns. for forming prepregs)

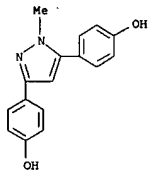
RN 43222-90-8 CAPLUS

CN 1H-Pyrazole, 3,5-bis(4-methoxyphenyl)-1-methyl- (9CI) (CA INDEX NAME)

L13 ANSWER 4 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 912804-13-8 CAPLUS
CN Phenol, 4,4'-(1-methyl-1H-pyrazole-3,5-diyl)bis- (9CI) (CA INDEX NAME)



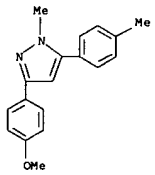
L13 ANSWER 5 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:660707 CAPLUS
DOCUMENT NUMBER: 145:292939
TITLE: Reaction of N-Monosubstituted Hydrazones with Nitroolefins: A Novel Regioselective Pyrazole Synthesis
AUTHOR(S): Deng, Xiaohu; Mani, Neelakandha S.
CORPORATE SOURCE: Department of Drug Discovery, Johnson & Johnson Pharmaceutical R & D LLC, San Diego, CA, 92121, USA
SOURCE: Organic Letters (2006), 8(16), 3505-3508 CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel regioselective synthesis of substituted pyrazoles from N-monosubstituted hydrazones and nitroolefins is described. The reaction is performed in a one-pot manner and the yields range from moderate to excellent. A key nitropyrazolidine intermediate is characterized and a plausible mechanism is proposed.

IT 908329-93-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(one-pot regioselective synthesis of substituted pyrazoles from N-monosubstituted hydrazones and nitroolefins)

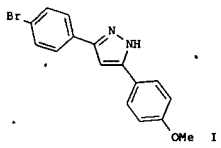
RN 908329-93-1 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-1-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 6 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN

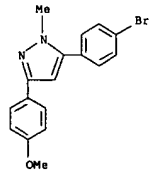
ACCESSION NUMBER: 2006:504334 CAPLUS
DOCUMENT NUMBER: 145:8083
TITLE: 1,3-Diketones from Acid Chlorides and Ketones: A Rapid and General One-Pot Synthesis of Pyrazoles
AUTHOR(S): Heller, Stephen T.; Natarajan, Swaminathan R.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Organic Letters (2006), 8(13), 2675-2678 CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:8083
GI



AB 1,3-Diketones were synthesized directly from ketones and acid chlorides and were then converted in situ into pyrazoles, e.g. I, by the addition of hydrazine. This method is extremely fast, general, and chemoselective, allowing for the synthesis of previously inaccessible pyrazoles and synthetically demanding pyrazole-containing fused rings.

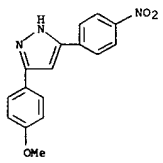
IT 888482-87-9P 888482-96-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazoles via 1,3-diketones from acid chlorides and ketones)

RN 888482-87-9 CAPLUS
CN 1H-Pyrazole, 5-(4-bromophenyl)-3-(4-methoxyphenyl)-1-methyl- (9CI) (CA INDEX NAME)



RN 888482-96-0 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

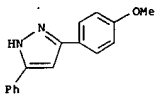
L13 ANSWER 6 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

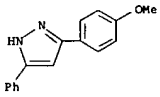
Karen Cheng

L13 ANSWER 7 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:281522 CAPLUS
DOCUMENT NUMBER: 144:468066
TITLE: A novel synthesis of 5-aryl-3-phenylpyrazole from 2-aryl-3-benzoyl-1,1-cyclopropanedicarbonitrile and hydrazine
AUTHOR(S): Ren, Zhongjiao; Cao, Weiguo; Chen, Jie; Wang, Yu; Ding, Weiyu
CORPORATE SOURCE: Department of Chemistry, Shanghai University, Shanghai, 200444, Peop. Rep. China
SOURCE: Journal of Heterocyclic Chemistry (2006), 43(2), 495-497
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new process for synthesis of 5-aryl-3-phenylpyrazole is achieved. The regioselective ring-opening reaction of 2-aryl-3-benzoyl-1,1-cyclopropanedicarbonitrile with hydrazine plays a crucial role in the described process. The structures of the pyrazoles were established on the basis of the spectroscopic anal and confirmed by the x-ray diffraction anal. of 3,5-diphenylpyrazole.
IT 32664-28-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and structure of 5-aryl-phenylpyrazoles from 2-aryl-benzoyl-cyclopropanedicarbonitrile and hydrazine hydrate)
RN 32664-28-1 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-5-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

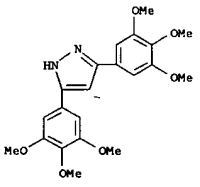
L13 ANSWER 8 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1299340 CAPLUS
DOCUMENT NUMBER: 144:191632
TITLE: Facile preparation of allyl amines and pyrazoles by hydrazinolysis of 2-ketoaziridines
AUTHOR(S): Chen, Gang; Sasaki, Mikio; Yudin, Andrei K.
CORPORATE SOURCE: Davenport Research Laboratories, Department of Chemistry, University of Toronto, Toronto, ON, M5S 3H6, Can.
SOURCE: Tetrahedron Letters (2005), Volume Date 2006, 47(3), 255-259
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:191632
AB Allyl amines and pyrazoles can be obtained by hydrazinolysis of 2-ketoaziridines. A variety of aziridines, including N-unprotected, N-substituted, as well as bicyclic enamine and aminal types, can be transformed into diversely substituted linear or cyclic products. The hydrazinolysis of homochiral aziridines proceeds without racemization.
IT 32664-28-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of allyl amines and pyrazoles by hydrazinolysis of 2-ketoaziridines)
RN 32664-28-1 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-5-phenyl- (9CI) (CA INDEX NAME)



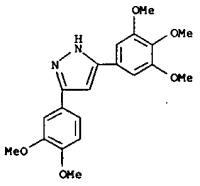
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 9 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1033793 CAPLUS
DOCUMENT NUMBER: 143:359448
TITLE: Synthesis and cytotoxicity of epoxide and pyrazole analogs of the combretastatins
AUTHOR(S): LeBlanc, Regan; Dickson, John; Brown, Toni; Stewart, Michelle; Pati, Hari N.; VanDerveer, Don; Arman, Hadi; Harris, Jeff; Pennington, William; Holt, Herman L.; Lee, Moses
CORPORATE SOURCE: Department of Chemistry, Furman University, Greenville, SC, 29613, USA
SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(21), 6025-6034
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:359448
AB Twenty-six epoxide and corresponding pyrazole derivs., of the structurally related chalcones and combretastatin A-4 (CA-4), were synthesized and tested for in vitro cytotoxicity. These mols. were synthesized by epoxidn. of the relevant chalcones, followed by reaction with hydrazine. The structures of 1 epoxides, and a pyrazole, were confirmed by x-ray diffraction studies. The relatively coplanar conformation of a 3',3'',4',4'',5',5''-hexamethoxypyrazole was in good agreement with the shape for 3',3'',4',4'',5'-pentamethoxypyrazole, which was determined from mol.
mechanics optimization. In vitro cytotoxicity of each class of compds. was obtained using a 72 h continuous exposure MTT assay against two murine cancer cell lines: B16 melanoma and L1210 leukemia. The effect of substitution in the A-ring is addressed: three methoxy groups vs. two, generally increased cytotoxicity across both cell lines. In the majority of cases, the pyrazoles are generally more active than the epoxides, with the most active, 5-(3''-amino-4''-methoxyphenyl)-3-(3',4',5'-trimethoxyphenyl)pyrazole, possessing an IC50 value of 5 and 2.4 μM (B16 and L1210, resp.). Due to their planar conformations, the pyrazoles are typically less active than the corresponding chalcones, which adopt angular conformations similar to CA-4. B-ring modifications confirmed that in general the amino compds. are more active than the corresponding nitro compds. Varying the number and orientation of methoxy groups on the A-ring did not produce any significant differences in toxicity in the cell lines studied.
IT 851729-28-7P 861881-81-4P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and cytotoxicity of epoxide and pyrazole analogs of combretastatins towards tumor cells)
RN 851729-28-7 CAPLUS
CN 1H-Pyrazole, 3,5-bis(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L13 ANSWER 9 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

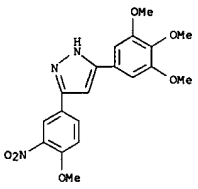


RN 861881-81-4 CAPLUS
CN 1H-Pyrazole, 3-(3,4-dimethoxyphenyl)-5-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

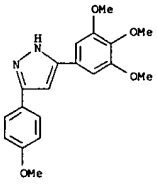


IT 866261-47-4P, 3-(3',4',5'-Trimethoxyphenyl)-5-(4'-methoxy-3'-nitrophenyl)pyrazole
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis and cytotoxicity of epoxide and pyrazole analogs of combretastatins towards tumor cells)
RN 866261-47-4 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxy-3-nitrophenyl)-5-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L13 ANSWER 9 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

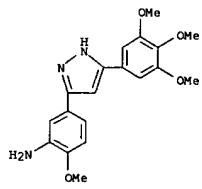


IT 851729-26-5P 866261-49-6P 866261-55-4P,
5-(3''-Amino-4''-methoxyphenyl)-3-(2',5'-dimethoxyphenyl)pyrazole
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and cytotoxicity of epoxide and pyrazole analogs of combretastatins towards tumor cells)
RN 851729-26-5 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-5-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

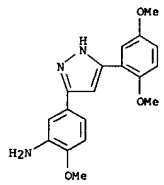


RN 866261-49-6 CAPLUS
CN Benzenamine, 2-methoxy-5-[5-(3,4,5-trimethoxyphenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L13 ANSWER 9 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

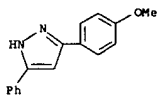


RN 866261-55-4 CAPLUS
CN Benzenamine, 5-[5-(2,5-dimethoxyphenyl)-1H-pyrazol-3-yl]-2-methoxy- (9CI) (CA INDEX NAME)

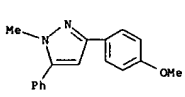


REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 10 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:952848 CAPLUS
DOCUMENT NUMBER: 143:405840
TITLE: One-Pot Construction of Pyrazoles and Isoxazoles with Palladium-Catalyzed Four-Component Coupling
AUTHOR(S): Ahmed, Mohamed S. Mohamed; Kobayashi, Kei; Mori, Atsunori
CORPORATE SOURCE: Chemical Resources Laboratory, Tokyo Institute of Technology, Yokohama, 226-8503, Japan
SOURCE: Organic Letters (2005), 7(20), 4487-4489
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:405840
AB Four-component coupling of a terminal alkyne, hydrazine (hydroxylamine), carbon monoxide, and an aryl iodide furnishes pyrazole or isoxazole derivs. in the presence of a palladium catalyst. The reaction proceeds at room temperature and an ambient pressure of carbon monoxide in an aqueous solvent system.
IT 32664-28-1P, 3-(4-Methoxyphenyl)-5-phenyl-1H-pyrazole
56119-91-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(one-pot construction of pyrazoles and isoxazoles by palladium-catalyzed four-component coupling)
RN 32664-28-1 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-5-phenyl- (9CI) (CA INDEX NAME)

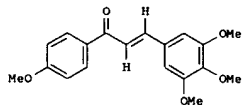


RN 56119-91-6 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-1-methyl-5-phenyl- (9CI) (CA INDEX NAME)

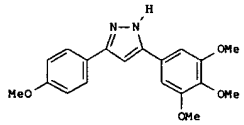


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 11 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:511399 CAPLUS
DOCUMENT NUMBER: 143:193943
TITLE: Synthesis and biological evaluation of chalcones and their derived pyrazoles as potential cytotoxic agents
AUTHOR(S): Bhat, B. A.; Dhar, K. L.; Puri, S. C.; Saxena, A. K.; Shanmugavel, M.; Qazi, G. N.
CORPORATE SOURCE: Division of Natural Product Chemistry, Regional Research Laboratory (CSIR), Jammu Tawi, 180001, India
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(12), 3177-3180
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:193943
GI



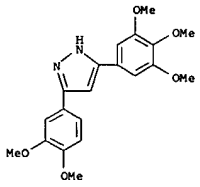
I



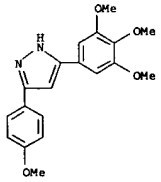
II

AB A series of substituted chalcones, e.g., I, and their corresponding pyrazoles, e.g., II, were synthesized and evaluated for in vitro cytotoxic activity against a panel of human cancer cell lines. Out of the compds. screened, 8 compds., showed marked activity. Some compds. were found to be the most promising in this study. SAR is also discussed.
IT 861881-81-4P
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation, anticancer activity, and structure-activity relationship of epoxychalcones, dihydrochalcones, dibromochalcones, and pyrazoles starting from chalcones)
RN 861881-81-4 CAPLUS
CN 1H-Pyrazole, 3-(3,4-dimethoxyphenyl)-5-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L13 ANSWER 11 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

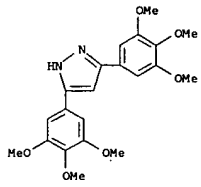


IT 851729-26-5P 851729-28-7P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, anticancer activity, and structure-activity relationship of epoxychalcones, dihydrochalcones, dibromochalcones, and pyrazoles starting from chalcones)
RN 851729-26-5 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-5-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)



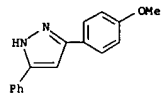
RN 851729-28-7 CAPLUS
CN 1H-Pyrazole, 3,5-bis(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L13 ANSWER 11 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

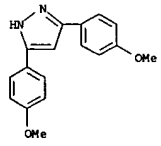


REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 12 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:359591 CAPLUS
DOCUMENT NUMBER: 142:463658
TITLE: Synthesis of 3,5-diphenyl-1H-pyrazoles
AUTHOR(S): Bhat, B. A.; Puri, S. C.; Qurishi, M. A.; Dhar, K. L.; Qazi, G. N.
CORPORATE SOURCE: Division of Natural Products Chemistry, Regional Research Laboratory (CSIR), Jammu Tawi, India
SOURCE: Synthetic Communications (2005), 35(8), 1135-1142
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Taylor & Francis, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:463658
AB An efficient and convenient synthesis of 3,5-diphenyl-1H-pyrazoles from chalcones by the action of hydrazine hydrate on chalcone-epoxide followed by simultaneous dehydration is reported.
IT 32664-28-1P 75059-30-2P 851729-26-5P
851729-28-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 3,5-diphenyl-1H-pyrazoles via epoxidn. of chalcones followed
by reaction of epoxides with hydrazine hydrate and dehydration)
RN 32664-28-1 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-5-phenyl- (9CI) (CA INDEX NAME)

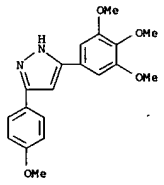


RN 75059-30-2 CAPLUS
CN 1H-Pyrazole, 3,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

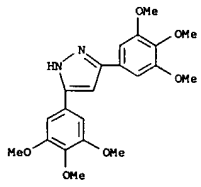


RN 851729-26-5 CAPLUS
CN 1H-Pyrazole, 3-(4-methoxyphenyl)-5-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L13 ANSWER 12 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 851729-28-7 CAPLUS
CN 1H-Pyrazole, 3,5-bis(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

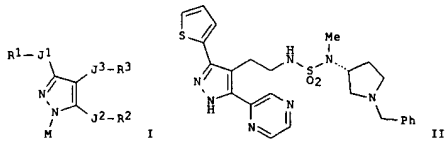


REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 13 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:284151 CAPLUS
DOCUMENT NUMBER: 142:355262
TITLE: Preparation of pyrazolyl inhibitors of 15-lipoxygenase
INVENTOR(S): Ngu, Khehyong; Weinstein, David S.; Robl, Jeffrey A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 48 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

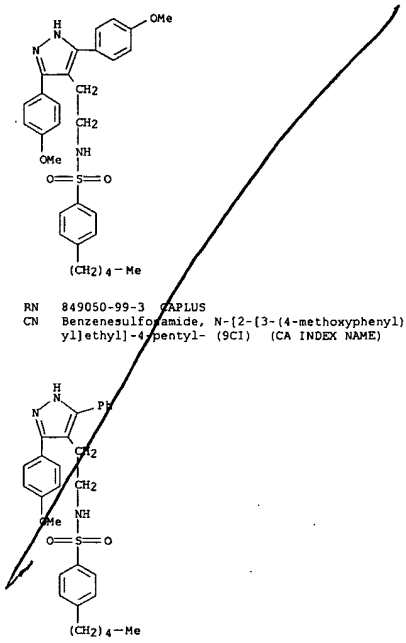
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005070589	A1	20050331	US 2004-932981	20040901
PRIORITY APPLN. INFO.:			US 2003-499498P P	20030902

OTHER SOURCE(S): CASREACT 142:355262; MARPAT 142:355262
GI



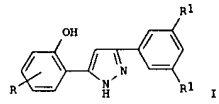
AB The title compds. I [J1, J2 = a bond, CO, OCO, CO2, etc.; J3 = (un)substituted alkenylene, cycloalkylene, alkenylene, etc.; M = H, alkyl, cycloalkyl, aryl, etc.; R1, R2 = H, alkyl, cycloalkyl, aryl, etc.; R3 = phthalimido, (un)substituted NHSO2Z, NHCOZ, etc.; Z = (un)substituted NH2, alkyl, cycloalkyl, etc.], useful for treating diseases related to the 15-LO cascade (no data), were prepared E.g., a multi-step synthesis of II, starting from 4-chloro-2'-butyrothienone, was given. The pharmaceutical composition comprising the compound I is claimed.
IT 849050-97-1P 849050-99-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrazoles for treating diseases related to the 15-LO cascade)
RN 849050-97-1 CAPLUS
CN Benzenesulfonamide, N-[2-[3,5-bis(4-methoxyphenyl)-1H-pyrazol-4-yl]ethyl]-4-pentyl- (9CI) (CA INDEX NAME)

L13 ANSWER 13 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

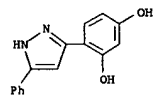


RN 849050-99-3 CAPLUS
CN Benzenesulfonamide, N-[2-[3-(4-methoxyphenyl)-5-phenyl-1H-pyrazol-4-yl]ethyl]-4-pentyl- (9CI) (CA INDEX NAME)

L13 ANSWER 14 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:38350 CAPLUS
DOCUMENT NUMBER: 142:463649
TITLE: Synthesis and antimicrobial activity of 3,5-diarylpyrazoles
AUTHOR(S): Prasad, Y. Rajendra; Prasanna, G. Lakshmi; Chakradhar, V.
CORPORATE SOURCE: Department of Pharmaceutical Sciences, Andhra University, Visakhapatnam, 530 003, India
SOURCE: Asian Journal of Chemistry (2005), 17(1), 621-623
CODEN: AJCHEW; ISSN: 0970-7077
PUBLISHER: Asian Journal of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:463649
GI

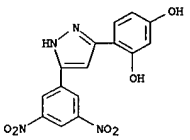


AB Title compds. I (R = 4-OH, 5-OH; R1 = H, NO2) were prepared by cyclocondensation of diaryl β-diketones with hydrazine hydrate. Antibacterial and antifungal activities of I were determined
IT 38214-70-9P 851676-89-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antibacterial and antifungal activity of diarylpyrazoles)
RN 38214-70-9 CAPLUS
CN 1,3-Benzenediol, 4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)



RN 851676-89-6 CAPLUS
CN 1,3-Benzenediol, 4-[5-(3,5-dinitrophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L13 ANSWER 14 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

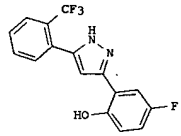
Karen Cheng

L13 ANSWER 15 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:780671 CAPLUS
DOCUMENT NUMBER: 141:296010
TITLE: Preparation of substituted pyrazoles as modulators of ATP-binding cassette transporters
INVENTOR(S): Vangoor, Frederick F.; Hadida Ruah, Sarah S.; Singh, Ashvani K.; Olson, Eric R.; Makings, Lewis R.; Gonzalez, Jesus E., III; Rader, James A.; Chambers, Fred, III; Miller, Mark T.; Grootenhuis, Peter; Liu, Yahua
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 174 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004080972	A1	20040923	WO 2004-US7492	20040312
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005113423	A1	20050526	US 2004-800022	20040312
EP 1601657	A1	20051207	EP 2004-720345	20040312
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
PRIORITY APPLN. INFO.:			US 2003-453978P	P 20030312
			WO 2004-US7492	W 20040312

OTHER SOURCE(S): MARPAT 141:296010
GI

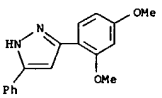
I



II

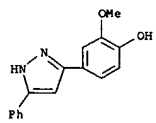
L13 ANSWER 15 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Pyrazoles I [A, B = (un)substituted aryl, heterocyclyl, cycloalkyl; C = H, (un)substituted aryl, heterocyclyl, heteroaryl, cycloalkyl, alkyl, alkylcarbonyl, arylcarbonyl, heteroarylcarbonyl, heterocyclylcarbonyl, or aminocarbonyl; X = H, (un)substituted alkyl, aryl, heterocyclyl, heteroaryl, or ω-substituted n-alkyl] such as II are prepared as inhibitors of ATP-binding cassette (ABC) transporters such as the cystic fibrosis transmembrane conductance regulator (CFTR) for use in the treatment of conditions such as cystic fibrosis, immunodeficiency, inflammatory disease, chronic obstructive pulmonary disease, chronic pancreatitis, or pneumonia. 4-Trifluoromethylbenzoyl chloride and 2-hydroxy-5-fluoroacetophenone are stirred in pyridine for 12 h, after which potassium hydroxide is added and the mixture stirred for 12 h; addition of hydrazine hydrate to a solution of the product obtained in the first step in ethanol and heating at reflux for 3 h yields II in 30% overall yield as a yellow crystalline solid. II modulates ΔF508-CFTR at ≥75% of the effect of genistein on the same receptor. Data on the relative modulation of ΔF508-CFTR by some compds. of the invention as compared to genistein is provided.
IT 763133-89-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrazoles as modulators of ATP-binding cassette transporters such as the cystic fibrosis transmembrane conductance regulator for treatment of diseases such as cystic fibrosis, immunodeficiency, and pneumonia)
RN 763133-89-7 CAPLUS
CN 1H-Pyrazole, 3-(2,4-dimethoxyphenyl)-5-phenyl- (9CI) (CA INDEX NAME)



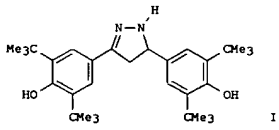
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 16 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:672993 CAPLUS
DOCUMENT NUMBER: 141:332112
TITLE: Resin-Bound 4H-1,3-Oxazine-Masked β-Diketones for Functionalizing Cleavage Strategy
AUTHOR(S): Vanier, Cecile; Wagner, Alain; Mioskowski, Charles
CORPORATE SOURCE: Faculte de Pharmacie, Laboratoire de Synthese Bio-Organique, Universite Louis Pasteur de Strasbourg, UMR 7514 Associee au CNRS, Illkirch, 67401, Fr.
SOURCE: Journal of Combinatorial Chemistry (2004), 6(5), 846-850
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:332112
AB Resin-bound 4H-1,3-oxazines are synthesized by the stepwise condensation of a resin-bound amide with an aldehyde and an alkyne. Starting materials used in this study included N-[Methoxy(4-methylphenyl)methyl]benzamide derivs. and alkynes, such as (ethynyl)benzene, (1-propynyl)benzene, 3,3-dimethyl-1-butyne, 3-phenyl-2-propynoic acid Et ester, etc. Upon DDQ activation, oxazines are converted into oxazinium salts. When treated with hydrazines, these resin-bound β-diketone equivalent yield pyrazoles through a functionalizing release process. This multicomponent capture strategy, tedious to handle in classical synthesis in solution, is well-suited to solid-supported chemical It facilitates the handling of sensitive and unstable intermediates, such as N-α-methoxyalkylamides and 1,3-oxazinium salts. For example, the reaction of Merrifield resin-bound N-[(methoxy)(phenyl)methyl]benzamide with (ethynyl)benzene gave a resin-bound 4,6-diphenyl-4H-1,3-oxazine (not isolated). Further reaction of this with hydrazine and functionalizing release gave 3,5-diphenyl-1H-pyrazole. A similar strategy also yielded 4,5,6,7-tetrahydro-3-phenyl-1H-indazole.
IT 773858-15-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrazole derivative using resin-bound 4H-1,3-oxazine-masked β-diketone for functionalizing cleavage strategy)
RN 773858-15-4 CAPLUS
CN Phenol, 2-methoxy-4-(5-phenyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

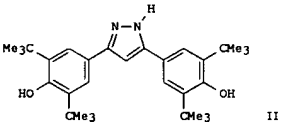


REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:362548 CAPLUS
DOCUMENT NUMBER: 141:106411
TITLE: Novel 3,5-diarylpyrazolines and pyrazole as low-density lipoprotein (LDL) oxidation inhibitor
AUTHOR(S): Jeong, Tae-Sook; Kim, Kyung Soon; Kim, Ju-Ryoung; Cho, Kyung-Hyun; Lee, Sangku; Lee, Woo Song
CORPORATE SOURCE: National Research Laboratory of Lipid Metabolism & Atherosclerosis, Korea Research Institute of Bioscience and Biotechnology, Daejeon, 305-333, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(11), 2719-2723
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:106411
GI



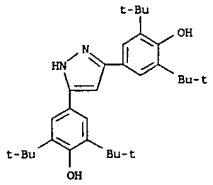
I



II

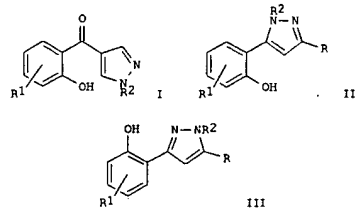
AB 2,3-Diarylpyrazolines, e.g., I, and -pyrazole II were synthesized by cyclocondensation of chalcones with hydrazine, and tested for their LDL-oxidation inhibition activity. The tested compds. showed significant LDL-antioxidant activities in the TBARS assay, the lag time of conjugated diene production, the relative electrophoretic mobility (REM) of ox-LDL, the apoB-100 fragmentation, and the macrophage-mediated LDL oxidation I and II were found to be the most active compds. as an inhibitor of LDL oxidation, and I (IC50 = 0.1 μM) was 6-fold more potent than probucol (IC50 = 0.6 μM) in the TBARS assay.
IT 721447-01-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and low-d. lipoprotein peroxidn. inhibition of bis[di(t-butyl)hydroxyphenyl]pyrazole via oxidation of bis[di(t-butyl)hydroxyphenyl]pyrazoline)

L13 ANSWER 17 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 721447-01-4 CAPLUS
CN Phenol, 4,4'-(1H-pyrazole-3,5-diyl)bis[2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 18 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:347011 CAPLUS
DOCUMENT NUMBER: 141:332110
TITLE: Design and synthesis of two pyrazole libraries based on o-hydroxyacetophenones
AUTHOR(S): Borrell, Jose I.; Schuler, Elisabeth; Teixido, Jordi; Michelotti, Enrique L.
CORPORATE SOURCE: Institut Quimic de Sarria, Grup d'Enginyeria Molecular, Universitat Ramon Llull, Barcelona, E-08017, Spain
SOURCE: Molecular Diversity (2004), 8(2), 147-157
CODEN: MODIF4; ISSN: 1381-1991
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:332110
GI

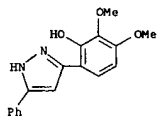


AB Two new solid-phase syntheses of substituted pyrazoles are described. The first includes supporting an o-hydroxyacetophenone on Merrifield resin, Vilsmeier-Haack formylation on the Me group and cyclization with a substituted hydrazine to afford a pyrazole ring with two diversity centers, e.g. I [R1 = H, 4-F, 3,4-(MeO)2, etc., R2 = Ph, n-Pr, 2-benzothiazolyl, etc.]. The second starts from o-hydroxyacetophenone supported on Wang resin, which undergoes a Claisen condensation with a carboxylic acid ester to yield a 1,3-dicarbonyl compound that cyclizes to a pyrazole using a hydrazine, II and III (R = H, Me, Ph). Both methods have been used to synthesize two small pyrazole libraries.
IT 771483-41-1P 771483-45-5P 771486-14-7P
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(design and solid-phase syntheses of pyrazole libraries using o-hydroxyacetophenones, their fungicidal, insecticidal, and herbicidal activities)
RN 771483-41-1 CAPLUS
CN Phenol, 2,3-dimethoxy-6-(5-phenyl-1H-pyrazol-3-yl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

L13 ANSWER 18 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 771483-40-0
CMF C17 H16 N2 O3



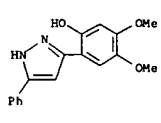
CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 771483-45-5 CAPLUS
CN Phenol, 4,5-dimethoxy-2-(5-phenyl-1H-pyrazol-3-yl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 771483-44-4
CMF C17 H16 N2 O3



CM 2

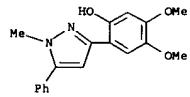
CRN 76-05-1
CMF C2 H F3 O2

L13 ANSWER 18 OF 96 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 771486-14-7 CAPLUS
CN Phenol, 4,5-dimethoxy-2-(1-methyl-5-phenyl-1H-pyrazol-3-yl)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 771486-13-6
CMF C18 H18 N2 O3



CM 2

CRN 76-05-1
CMF C2 H F3 O2

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT